Rapid Communications

Vortex lattice in two-dimensional chiral XY ferromagnets and the inverse Berezinskii-Kosterlitz-Thouless transition

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In this Rapid Communication we will show that, in the presence of a properly modulated Dzyaloshinskii-Moriya (DM) interaction, a $U(1)$ vortex-antivortex lattice appears at low temperatures for a wide range of the DM interaction. Even more, in the region dominated by the exchange interaction, a standard Berezinskii-Kosterlitz-Thouless (BKT) transition occurs. In the opposite regime, the one dominated by the DM interaction, a kind of inverse BKT transition takes place. As temperature rises, the vortex-antivortex lattice starts melting by the annihilation of vortex-antivortex pairs, in a sort of "inverse" BKT transition.

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Motivation. Since the seminal works from Berezinskii, Kosterlitz, and Thouless (BKT) [1–3], the BKT transition (a topological defect-mediated phase transition) and the existence of $U(1)$ vortices in the disordered phase of two-dimensional (2D) Heisenberg XY ferromagnets have disruptively influenced the physics of condensed matter, giving topology a central role in the physics beyond the Landau paradigm. The existence of periodic arrangements of these topologically singular excitations [$U(1)$ vortices], on the other hand, is also very well established both from theoretical and experimental points of view, and they have played a central role in condensed matter since they were postulated by Abrikosov in 1957 [4], and observed in type-II superconductors 10 years later by Essmann and Träuble [5]. These $U(1)$-vortex lattices appear in many different materials, from high critical temperature (HTC) superconductors to ^{4}He superfluids, and BECs, or in the so-called fully frustrated XY model (FFXY) used to model periodic arrays of Josephson junctions [6–11]. Nevertheless, the existence of such lattices as stable states of two-dimensional pure magnetic materials is not so well known.

In the past years, a new kind of magnetic materials, known as chiral magnets, has captured the attention of the condensed matter community, due to their capability for supporting periodic arrangements of another type of topologically nontrivial magnetic excitation, in this case, a smooth kind of topological excitation named skyrmions, relevant for memory devices and quantum computing technology. The key ingredient to stabilize these lattices seems to be chirality. In these magnets, it is widely assumed that this chirality is a consequence of an antisymmetric exchange interaction, the Dzyaloshinskii-Moriya (DM) interaction, originated in the spin-orbit coupling of noncentrosymmetric magnetic materials. The technological implication of these chiral magnets, and in particular of the skyrmion crystal phases they support, has motivated a race for the enhancement and modulation of the DM interaction by different methods, leading to the emergence of a new research field named "spin orbitronics"[12]. Recent studies show that in carefully designed heterostructures of chiral magnets, and by the proper application of electric fields, among other techniques, it is possible to achieve DM interactions of the same order of magnitude as the exchange one [12–14]. Also, it has been shown that the DM magnitude could grow linearly with the applied electric fields and can also be modulated [12], opening new technological possibilities.

In this context, we will revisit the XY models for ferromagnets, now in the presence of strong DM interactions. We will show in this Rapid Communication that for values of the DM interaction slightly stronger than the exchange interaction, a vortex-antivortex lattice can be stabilized at low temperatures. Even more surprisingly, in the region dominated by the DM interaction, the system undergoes a finite-temperature phase transition in the same universality class as the BKT transition. By mapping the system to a 2D Coulomb gas, we interpret this transition as a sort of inverse BKT transition (iBKT), in which the vortex lattice starts melting, as the temperature rises, by the annihilation of vortex-antivortex pairs. In what follows, we derive the results leading to this conclusion.

Model. We will start by considering a ferromagnetic XY Hamiltonian in the presence of an antisymmetric DM interaction on a square two-dimensional lattice,

$$\mathcal{H} = -\sum_{\mathbf{r}_i,\hat{\mu}} J_{i\hat{\mu}} \mathbf{S_i} \cdot \mathbf{S}_{\mathbf{i}+\hat{\mu}} + \mathbf{D}_{\mathbf{i}\hat{\mu}} \cdot (\mathbf{S_i} \times \mathbf{S}_{\mathbf{i}+\hat{\mu}}), \tag{1}$$

where $\hat{\mu}$ represents the unit vectors along positive axis directions, the spin $\mathbf{S}$ is a two-component unimodular vector, $J > 0$ is the ferromagnetic exchange coupling, and the $\mathbf{D}_{i\hat{\mu}}$ vectors pointing outside the plane of the lattice (let us say the XY plane) represent the DM interaction.

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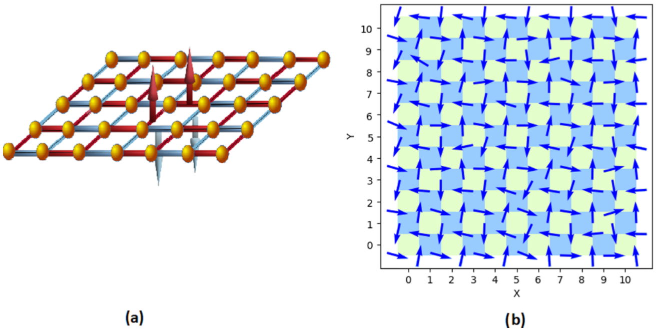

FIG. 1. (a) shows the direction of the D vectors, represented by red and light blue out-of-plane arrows of a given plaquette, when circulating the lattice in the positive direction of the axes. The colors of the bonds indicate the corresponding directions for the remaining D vectors. (b) shows a vortex lattice of 10×10 spins obtained through a standard Metropolis Monte Carlo method, where the X and Y axes represent the direction on the lattice in units of the lattice spacing. Green plaquettes hold a counterclockwise vortex while blue plaquettes hold a clockwise vortex, and spins in each sites are represented with blue arrows.

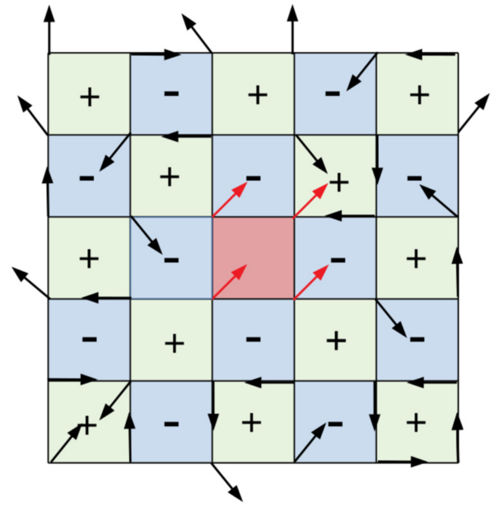

FIG. 2. Illustrative: The figure shows a configuration in which only one vortex, a positive one, has been eliminated from the lattice, and the remaining vortex-antivortex lattice has not been affected; D-dominated regime.

We define new variables $\varphi_{i,\hat{\mu}}$ and $\mathcal{J}_{i,\hat{\mu}}$, in terms of which the original variables read $J_{i,\hat{\mu}} = \cos(\varphi_{i,\hat{\mu}})\mathcal{J}_{i,\hat{\mu}}$ and $D_{i,\hat{\mu}} = \sin(\varphi_{i,\hat{\mu}})\mathcal{J}_{i,\hat{\mu}}$, and the Hamiltonian can be recast in the following way,

$$\mathcal{H} = -\sum_{\mathbf{r_i},\hat{\mu}} \mathcal{J}_{i,\hat{\mu}} \cos(\theta_i - \theta_{i+\hat{\mu}} - \varphi_{i,\hat{\mu}}), \tag{2}$$

where θ_i represents the angle with respect to a given fixed direction of the $\mathbf{S}_i$ vector. This Hamiltonian has been previously studied by Teitel and collaborators in the context of Josephson junction arrays (see, for example, Ref. [11] and references therein), showing that it supports a vortex lattice at low temperatures. The φ configuration that will be studied here explicitly breaks the $\mathbb{Z}_2$ symmetry present in the models studied by Teitel, and the phenomenology derived from it, as far as we know, has not been previously reported [15]. The stable configurations, of course, will depend on the particular field configuration $\varphi_{i,\hat{\mu}}$ chosen. A simple nontrivial choice for $\varphi_{i,\hat{\mu}}$ corresponds to a constant value, $|\varphi_{i,\hat{\mu}}| = \varphi$, with alternating signs along the bonds, as depicted in Fig. 1(a). This φ configuration, the only one that we consider here [16], leads to a lattice of *minimal vortices* [17]. The energy condition imposed by Hamiltonian (2) for a given plaquette with D vectors pointing down along the lower and right bonds and pointing up in the other two bonds reads

$$\begin{aligned} 0 &= \sin\left(\frac{2\theta_1 - \theta_2}{2}\right)\cos\left(\frac{\theta_2 - 2\varphi}{2}\right), \\ 0 &= 2\sin\left(\frac{2\theta_2 - \theta_1 - \theta_3}{2}\right)\cos\left(\frac{\theta_3 - \theta_1 - 2\varphi}{2}\right), \\ 0 &= 2\sin\left(\frac{2\theta_3 - \theta_2}{2}\right)\cos\left(\frac{\theta_2 + 2\varphi}{2}\right), \end{aligned} \tag{3}$$

where a possible global phase has been set to zero, because of $U(1)$ global invariance. The angles $\theta_1, \ldots, \theta_4$ are numerated counterclockwise starting at the lower left-hand corner of the plaquette. Ferromagnetic and counterclockwise vortex configurations with $\Delta\theta_{i+1,i} = \pi/2$ satisfy the condition (3) for any value of φ, with the corresponding energies

$$E_f = -4\cos(\varphi), \tag{4a}$$

$$E_v = -4\cos(\pi/2 - \varphi). \tag{4b}$$

It is straightforward to check that the four adjacent plaquettes (two corners sharing) to the one considered, have the same both trivial and nontrivial solutions with the same energies, but with a clockwise vortex instead of anticlockwise. That means that for $\varphi \in [0, \frac{\pi}{4})$ the ground state becomes ferromagnetic, while for $\varphi \in (\frac{\pi}{4}, \pi/2]$ a vortex-antivortex lattice is stabilized, as in Fig. 1(b). The high symmetry in Fig. 1(b) can lead us to mistakenly conclude that a plaquette surrounded by four plaquettes with vortices of one type only admits a vortex of the opposite type. The illustrative Fig. 2 can clarify this aspect. Finally, for $\varphi = \frac{\pi}{4}$ the possibility of a coexistence of both phases cannot be discarded [18].

Low-temperature effective theory. We will start the analysis of the system by performing a low-temperature expansion following Savit [19]. We notice that $\mathcal{J}_{i,\hat{\mu}}$ is independent of bond and lattice site, and representing $\varphi_{i,\hat{\mu}}$ as a vector $\boldsymbol{\varphi}_i$ with components $\varphi_{\hat{x},i} = (-1)^{x_i+y_i}\varphi$ and $\varphi_{\hat{y},i} = (-1)^{x_i+y_i+1}\varphi$ on each site i, the partition function associated with the Hamiltonian (2) can be written as

$$Z = \int_{-\pi}^{\pi} \prod_j \frac{d\theta_j}{2\pi} \exp\left[\beta\mathcal{J}\sum_{i,\mu}\cos(\theta_i - \theta_{i+\mu} - \boldsymbol{\varphi}_i \cdot \hat{\mu})\right]. \tag{5}$$

Expanding each exponential in a series of Bessel functions [20], this partition function can be recast as

$$Z = \sum_{\{n\}} \left(\prod_{i,\mu} I_{n_{i,\mu}}(\beta \mathcal{J}) \exp[-i n_{i,\mu} \boldsymbol{\varphi}_i \cdot \hat{\mu}] \right) \times \int_{-\pi}^{\pi} \left(\prod_j \frac{d\theta_j}{2\pi} \right) \exp\left[\sum_{i,\mu} i n_{i,\mu} (\theta_i - \theta_{i+\mu}) \right], \quad (6)$$

where $\{n\}$ represents a sum over all possible integer configurations, one $n_{i,\mu}$ per bond, and $I_n(\beta\mathcal{J})$ are the modified Bessel functions of the first kind of order n. In this factorized way, integration over each angular variable can be done, and a theory on the discrete variable n, with the condition

$$\boldsymbol{\Delta} \cdot \mathbf{n}_i = n_{i,x} - n_{i-\hat{x},x} + n_{i,y} - n_{i-\hat{y},y} = 0, \quad (7)$$

is obtained. Of course, this null discrete divergence condition can be immediately fulfilled by a discrete rotor $n_{j,\mu} = \epsilon_{\mu\nu}\Delta_\nu \phi_j$, where $\{\phi\}$ is a set of integers defined on the dual lattice, that is, the square lattice formed by the center of the original plaquettes. Introducing Dirac's deltas, $\sum_{k=-\infty}^{\infty} \delta(\phi - k) = \sum_{m=-\infty}^{\infty} e^{i2\pi m_j \phi_j}$, the sum over discrete variables can be turned into integrals of now continuous ϕ_j and, at sufficient low temperature, the low-energy partition function can be written as

$$Z = \int \mathcal{D}\phi \sum_{\{m\}} \exp\left[\sum_{\mu,j} -\frac{1}{2\beta\mathcal{J}} (\Delta_\mu \phi_j)^2 + i2\pi M_j \phi_j \right], \quad (8)$$

where $M_j = m_j - (-1)^{x_j+y_j} \frac{2\varphi}{\pi}$ has been introduced.

Performing the Gaussian integrals by Fourier transforming the fields, the partition function reads

$$Z = Z^0 \sum_{\{m\}} \exp\left[-\frac{\beta\mathcal{J}}{8} \sum_{i,j} M_i V_{ij} M_j \right], \quad (9)$$

where

$$Z^0 = \exp\left[-\int_{-\pi}^{\pi} d^2q \frac{1}{2} \ln\left(\frac{2K(q)}{\pi} \right) \right],$$
$$V_{ij} = \int_{-\pi}^{\pi} d^2q \frac{e^{i\vec{q}(\vec{i}-\vec{j})}}{\left(1 - \frac{1}{2}\sum_\mu \cos(\vec{q}\cdot\hat{\mu})\right)}, \quad (10)$$

with $K(q)$ approximated by

$$K(q) = \frac{1}{2\beta\mathcal{J}\pi^2} \left(1 - \frac{1}{2} \sum_\mu \cos(\vec{q}\cdot\hat{\mu}) \right).$$

For small $|q|$ the potential reduces to the Coulomb gas potential, $V_{ij} \simeq \int_{-\pi}^{\pi} 2\frac{e^{iq(i-j)}}{|q|^2} d^2q$, that, after proper regularization by imposing charge neutrality $\sum_i M_i = 0$ [21], leads to the low-temperature partition function,

$$Z = Z^0 \sum_{\{m\}} \exp\left[\beta\mathcal{J}\pi \sum_{i,j} M_i \ln(|\mathbf{R}_i - \mathbf{R}_j|) M_j - \beta\mathcal{J}\pi \sum_l \left(\frac{1}{2}\ln(8) + \gamma \right) M_l^2 \right], \quad (11)$$

where γ is the Euler-Mascheroni constant.

This low-temperature effective theory is, in fact, an extension of the well-known description of the XY model ($\varphi = 0$) as a two-dimensional Coulomb gas [19,22].

It is clear now that the system at low temperatures can be understood as a neutral Coulomb gas of excitations of charges M, regardless of the value of φ. More precisely, at each value of φ the ground state of the system corresponds to a configuration in which the charges M take their minimal possible absolute value. It is interesting to note that, both in a pure exchange regime and in a pure DM regime, the charges become an integer and the minimal possible values for M correspond to $M_i = 0, \forall i$. In the pure exchange regime, $\varphi \to 0$, the charge $M_i = m_i$, where m_i represents the ith topological charge in the low-temperature theory [19]. The condition $M_i = 0, \forall i$ implies that no topological excitation is present at sufficiently low temperatures, as expected for a ferromagnetic ground state, Eq. (4). On the other hand, in the pure DM regime, $\varphi \to \frac{\pi}{2}$, the charge becomes $M_i = m_i - (-1)^{x_i+y_i}$. The condition $M_i = 0, \forall i$ implies that $m_i = (-1)^{x_i+y_i}$ at each site, and a fully populated vortex-antivortex lattice emerges at a sufficiently low temperature, again as expected from the microscopical theory, Eq. (4). At any intermediate value of φ, the condition that $|M|$ must be the minimal possible shows that the ferromagnetic background extends to all the region dominated by the exchange interaction, and the vortex-antivortex lattice background extends to all the region dominated by the DM interaction, also as predicted by the microscopic theory. The relevance of the effective theory relies on the interpretation of the excitations at low temperature. The study of the excitations in the microscopical theory could be very cumbersome, and the effective theory can shed some light on this matter. Excitations correspond to values of the charges different from their minimal values, and behave as a neutral Coulomb gas. On the exchange-dominated regime, the minimal energy excitation corresponds to one pair of nonminimal charges $M = \pm\mu$, which implies that a pair of one vortex and one antivortex has been created, i.e., $m = \pm 1$, and the well-known phenomenology of the XY model follows. Very interesting features not present in the standard XY model appear for $\varphi < \pi/4$, but they will be discussed in a forthcoming paper. In this Rapid Communication we will discuss the phenomenology in the DM-dominated regime.

DM-dominated regime and helicity modulus. As we have already mentioned, in the DM-dominated regime the ground state corresponds to a regular arrangement of vortices and antivortices, as depicted in Fig. 1(b). This can be seen from the minimal charge condition for $M_j = m_j - (-1)^{x_j+y_j}\frac{2\varphi}{\pi}$, for $\frac{2\varphi}{\pi} > \frac{1}{2}$. Regardless of the value of $\varphi > \pi/4$, the minimal condition is achieved by $m_j = (-1)^{x_j+y_j}$. Again, the minimal excitation is given by one pair of nonminimal opposite charges $M = \pm\mu$, but in this case it corresponds to $m = 0$ in both charges [23]. That is to say, the minimal excitation corresponds to a pair of opposite charges that now have a trivial winding number, one where before there was a vortex, and another one where before there was an antivortex, or rephrasing, the excitation corresponds to the annihilation of a pair of a vortex and an antivortex. This conclusion is not easy to reach from the microscopical theory since, although difficult, configurations with only one annihilated vortex can be constructed (see the illustrative Fig. 2). On the effective theory, on the other hand, it is an immediate conclusion from the neutrality charge. We notice that the "effective charge" oscillates with the position in such a way that it is not possible to move only one charge without violating charge neutrality.

As the temperature starts to rise, more pairs of opposite charges are created (more vortex-antivortex pairs are annihilated) and eventually, at some temperature, they could decouple and decorrelate the systems much in the same way as the vortices do in the XY model. We remark here that, although the transition shares many aspects with the BKT transition, the melting of the lattice goes in a direction inverse to the one in the BKT transition. In the present case, the system goes from topologically nontrivial entities in the stable state, to a decorrelated state dominated by topologically trivial excitations, so that we call this transition the inverse BKT transition (iBKT). In order to support this picture, we compute the helicity modulus, as it is standard in the BKT transition, and show that the iBKT transition has the same universal jump as the standard BKT transition, and numerically show that vortices are annihilated by pairs. The introduction of a λ_0 long-wavelength "twist" on the local order parameter, with $k_0 = 2\pi/\lambda_0$, should raise the free energy by $O(k_0^2)$ over their ground-state value, if the system is correlated, and should have no appreciable effect if the system is not [24]. That is to say, the helicity modulus Υ [25],

$$\Upsilon \equiv \left.\frac{\partial^2 F(T,k_0)}{\partial k_0^2}\right|_{k_0=0}, \tag{12}$$

where $F(T,k_0) = -T\ln[Z(\Phi,T)]/N$ is the free energy per unit volume, must be finite if the system is in the correlated phase and zero if it is not. In fact, the BKT transition is characterized by a finite jump in Υ/T_c of $2/\pi$. In what follows, we will show the numerical results for the helicity (12) for all values of the couplings and theoretical computations of the helicity modulus, following Ohta and Jasnow [24] (see Supplemental Material [27]), for extreme values of the parameters.

Helicity and phase transition. The Kosterlitz-Thouless renormalization group equations show that the helicity modulus Υ of a system of infinite size has a universal jump from the value $(2/\pi)T_c$ to zero at the critical temperature T_c. In Fig. 3, the behavior of Υ as a function of the temperature is shown for different values of D/J, where an abrupt jump in the helicity modulus at sufficiently high temperatures is observed. These results were obtained by a standard Metropolis Monte Carlo method with periodic boundary conditions on a square lattice of 32×32 sites. For extreme values, the theoretical prediction of the helicity in the correlated phase is also shown. We also compute numerically the positive and negative vortex densities for different values of D/J and we observe that, as temperature rises, both densities decrease at the same time, which implies that the vortices are annihilated by pairs. In Fig. 4, both densities as a function of the temperature are shown for $J = 0$. At each calculated temperature the densities have the same value. This is a nontrivial numerical result that coincides with the neutrality charge condition of the effective theory and rules out the possibility depicted in Fig. 2. The behavior of Υ is the one qualitatively expected for a BKT transition. The softening observed in the figure is due to the finite-size effect of the sample. Using the solution to

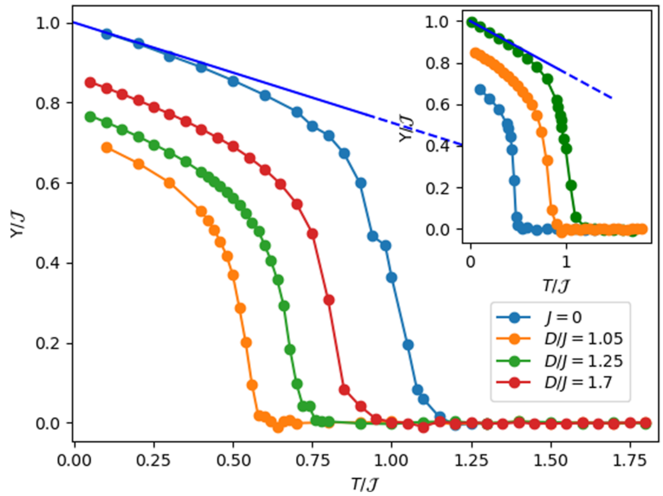

FIG. 3. The BKT behavior of $\Upsilon(T)$ for the chiral XY model in the D-dominated regime is shown. A jump in Υ is appreciated at each value of $\mathcal{J}$, and the theoretical prediction for $J \to 0$ is shown in purple. In the inset, the characteristic XY $\Upsilon(T)$ behavior for the J-dominated regime is also shown, and the curves with a lower intercept correspond to lower values of D/J.

the Kosterlitz-Thouless renormalization group equations and the 2D Coulomb gas duality, it has been shown that BKT transitions obey a particular scaling law with the sample size, that allows us to determine the transition temperature T_c [26],

$$\frac{\Upsilon(N,T)}{T\mathcal{J}} = \frac{\Upsilon^{\infty}(T)}{T\mathcal{J}}\left(1 + \frac{1}{2}\frac{1}{\ln(N) + C}\right), \tag{13}$$

where $\Upsilon(N,T)$ is the helicity modulus of the square lattice of N sites, C is an undetermined constant, and $\Upsilon^{\infty}(T)$ is the helicity modulus in the limit of $N \to \infty$. If the system undergoes a Kosterlitz-Thouless transition at a temperature T_c, we should obtain $\Upsilon^{\infty}(T_c)/(\mathcal{J}T_c) = 2/\pi$.

For the determination of T_c in the $D \gg J$ case, we follow the strategy developed by Weber and Minnhagen [26]. We calculate $\Upsilon(N,T)$ for lattice sizes ranging from 32×32

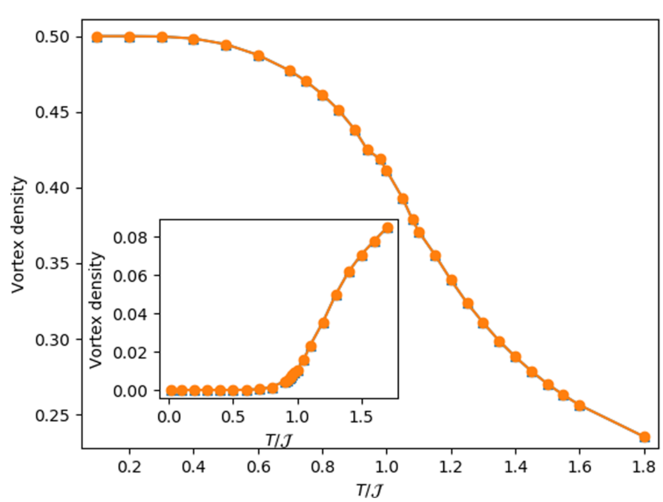

FIG. 4. The picture shows vortex and antivortex densities as temperature rises, for $D \gg J$. In the inset, the same densities show that standard phenomenology for $D = 0$.

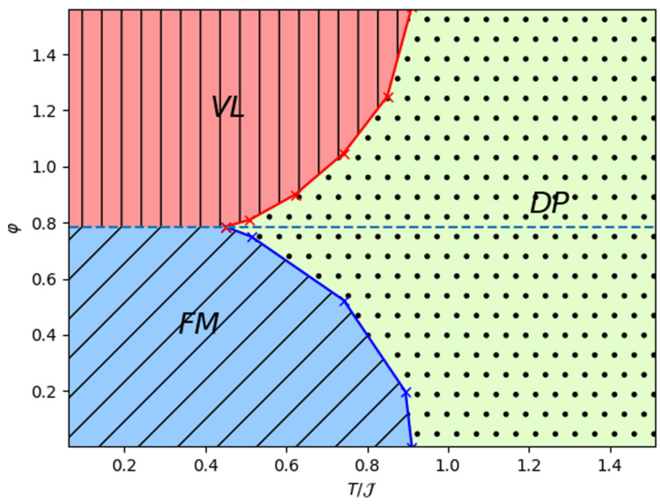

FIG. 5. Qualitative phase diagram of the studied model. The vertical axis represents the variable φ that goes from $\varphi = 0$ (J-dominated regime) up to $\varphi = \pi/4$ (D-dominated regime). The value $\varphi = \pi/4$ (where $D = J$) is depicted with a dashed horizontal line. We identify three regions: The region VL where the system stays in a vortex lattice configuration, the FM where the system stays in a ferromagnetic configuration, and the decorrelated high-temperature phase. As mentioned in the text, the possibility of a coexistence of both VL and FM phases at the dashed line cannot be discarded.

to 128×128 and temperatures ranging from $T = 0.885D$ to $T = 0.91D$. For a given T, we make a least-squares fit of $\Upsilon(N, T)/T$ to (13). We find that the quantity Υ^{∞}/T lies in the interval $0.61 < \Upsilon^{\infty}/T < 0.65$ for $0.885 < T/D < 0.9$. By this method Υ^{∞}/T_c is determined to be $\Upsilon^{\infty}/T_c = 2/\pi \pm 0.03$ and we can estimate T_c to be $T_c = 0.892(8)D$. For completeness, we include a qualitative phase diagram shown in Fig. 5.

We conclude that when $D \gg J$, the system undergoes a finite-temperature phase transition with the same universal jump as the BKT transition, but now mediated by topologically trivial excitations. In the extreme DM-dominated regime, it is not difficult to show that the charge-charge correlation function decays exponentially with temperature [27] and became less sensitive to charge positions, exactly in the same way that the vortex-antivortex correlation function does, and therefore a decoupling of the neutral pair of topologically trivial excitations is expected at a sufficiently high temperature. The existence of a vortex-antivortex lattice, and the iBKT transition it suffers, are the main results of this work.

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[16] By proper modulation of the DM interaction, lattices of vortices of arbitrary sizes can be built with the same tessellation technique.
[17] In this discrete context we will call a vortex, centered in a given plaquette, to every configuration of the order parameter $\theta(\mathbf{r_i})$ that, when circulating around the center of the plaquette, accumulates an integer times of 2π's, in steps smaller than π. A minimal vortex then is a vortex of the minimal size, i.e., a vortex of the size of the plaquette. This kind of vortex has been considered widely in the literature (see, for example, Ref. [11] and references therein).
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numerically we observe that as the temperature rises, the vortex density only decreases.

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